Metal-to-insulator transition and threshold electric field for SDW depinning in $(\text{TMTSF})_2\text{X}$ under pressure

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Abstract

Metal-to-insulator transition temperature (T_{MI}) and the activation energy (E_{A}) in the SDW phase of $(\text{TMTSF})_2\text{AsF}_6$ and $(\text{TMTSF})_2\text{PF}_6$ were determined under pressure. Pressure dependence of $2E_{\text{A}}/k_{\text{B}}T_{\text{MI}}$ near the critical pressure of the SDW phase, is compared with the mean-field theory by Yamaji. It was found that T_{MI} is not equal to the normal-to-SDW transition temperature but lower than T_{SDW} . Non-linear conduction was observed in a narrow temperature range above T_{MI} .

Introduction

In $(\text{TMTSF})_2\text{AsF}_6$ and $(\text{TMTSF})_2\text{PF}_6$ the spin density wave (SDW) state has been observed below $T_{\text{SDW}} \sim 10^1$ K at the ambient pressure. T_{SDW} is lowered under pressure. Brusetti et al. [1] showed from conductivity measurement that, in $(\text{TMTSF})_2\text{AsF}_6$, $T_{\text{SDW}}=12$ K at the ambient pressure and that the critical pressure P_{C} of the SDW phase is ~ 10.5 kb. Takahashi et al. [2] performed ^1H -NMR experiment in $(\text{TMTSF})_2\text{PF}_6$ under pressure and found that the SDW gap parameter at $T=0$, $\Delta_0(T=0)$, is insensitive to pressure while T_{SDW} is lowered with pressure. Their results are in good agreement with the mean-field theory first developed by Yamaji [3].

In the simplified model of electrons in $(\text{TMTSF})_2\text{X}$, a finite transverse transfer energy t_{b} is added to the one-dimensional dispersion. The Fermi surface is open but warped. In such a system, the ground state is the SDW and the energy gap develops over the entire area of the Fermi surface as long as t_{b} is smaller than the critical value. In the SDW state the band edges above and below the Fermi level are not constant but are modulated with amplitude ϵ_0 , where $\epsilon_0 \propto t_{\text{b}}^2$ is the measure of imperfect nesting of the Fermi surface. The SDW state is stabilized as long as ϵ_0 is smaller than the gap parameter at 0 K, $\Delta_0(T=0)$. While $\Delta_0(T=0)$ itself is insensitive to ϵ_0 , the SDW transition temperature T_{SDW} decreases with increasing ϵ_0 . The thermal activation energy E_{A} is equal to $\Delta_0(0) - \epsilon_0$ which is the minimum energy between occupied and unoccupied bands; it decreases with increasing ϵ_0 . Therefore, E_{A} is a useful parameter of the degree of imperfectness of the Fermi surface or the two-dimensionality of the system. Yamaji predicted that the semimetallic SDW state appears above $T_{\text{MI}} < T_{\text{SDW}}$ and that the temperature difference $T_{\text{SDW}} - T_{\text{MI}}$ increases with increasing ϵ_0 . From numerical calculation, Yamaji obtained that, as $\epsilon_0 \rightarrow \Delta_0$ ($E_{\text{A}} \rightarrow 0$), $2E_{\text{A}}/k_{\text{B}}T_{\text{SDW}} \rightarrow 0$ and $2E_{\text{A}}/k_{\text{B}}T_{\text{MI}} \rightarrow 1.4$, respectively.

Because it is expected that ϵ_0 increases with increasing the applied pressure, theoretical predictions have been compared with experimental results under pressure. We determined T_{MI} and E_{A} from ohmic conductivity under pressure. The

experimental results, especially the ratio $2E_A/k_B T_{MI}$ around P_C , are compared with the mean-field theory to determine whether T_{MI} is equal to or different from T_{SDW} . In addition, observation of non-linear conductivity in the temperature range near T_C is reported and discussed.

Experiment

Single crystals of $(TMTSF)_2AsF_6$ and $(TMTSF)_2PF_6$ were grown by the standard electrochemical method. Annealed gold wires of 10 μm diameter were used as electrical leads. They were attached with silver paste to Au pads evaporated on the sample. The current contacts covered the whole areas of both ends of the crystal for uniform current density. Mixture of kerosene and transformer oil with a ratio 1:1 was used as pressure medium in a clamp type bomb. In this experiment we have not observed resistance jump which frequently occurs during cooling at the ambient pressure.

We determined the T-P diagram below 4.2 kb from the superconducting transition temperature of indium manometer inside the bomb. Above 5kb, the actual pressure was estimated from the phase diagram of $(TMTSF)_2AsF_6$ determined by Brusetti et al. [1]. The metal-insulator transition temperature T_{MI} was determined from the peak of $|d(\ln \sigma_o)/d(1/T)|$ vs T curve, where σ_o is the ohmic conductance. The activation energy (E_A) was determined from the Arrhenius plot of σ_o below 2 K, i.e., below $T_C/2$ and $2E_A/3$ at the highest pressure in this work. Because of the non-linear increase of the conductivity in the SDW state, we measured the pulse conductivity and compared with the dc conductivity to determine σ_o .

Result and discussion

The ohmic conductance σ_o was measured carefully by repeated cooling and heating cycles, to find limit of temperature difference between the sample and the thermometer attached to the bomb. The values of T_{MI} determined from the heating and cooling runs were in agreement with each other within ± 0.2 K. The limit of uncertainty of E_A is smaller than $\pm 5\%$. The applied pressure was increased from 1 kb up to 9 kb and then decreased down to 1.5 kb. There was no hysteresis with changing pressure in the E_A - T_{MI} curve and the peak height of $|d(\ln \sigma_o)/d(1/T)|$ -T curve was reproducible. As shown in Fig.1 that peak is progressively broadened with pressure but does not vanish even at the highest pressure of $P \sim 9$ kb, in contrast with the results by Brusetti et al.[1] who could not observe the peak above 8 kb.

In both $(TMTSF)_2AsF_6$ and $(TMTSF)_2PF_6$, both T_{MI} and E_A decrease with increasing pressure. From Fig.2, the pressure coefficients of T_{MI} and E_A of $(TMTSF)_2AsF_6$ are $dT_{MI}/dP = -0.83$ K/kb and $dE_A/dP = -2.1$ K/kb below 4 kb, respectively. We have not determined T_{MI} of $(TMTSF)_2AsF_6$ at the ambient pressure directly. From extrapolation to $P=0$, $T_{MI}(P=0)=13.0$ K. These values should be compared with $dT_{MI}/dP \sim -0.6$ K/kb and $T_{MI}(P=0) \sim 12$ K obtained by Brusetti et al.[1] in $(TMTSF)_2AsF_6$.

In Fig.3 the ratio $2E_A/k_B T_{MI}$ is plotted, not against pressure, but against E_A because it is more convenient to compare the present results with the mean-field theory. From extrapolation to $P=0$, $2E_A/k_B T_{MI}$ in both $(TMTSF)_2AsF_6$ and $(TMTSF)_2PF_6$ at the ambient pressure is ~ 3.0 , which is much smaller than 3.53 expected from the mean-field theory when $\epsilon_o=0$. With decreasing E_A , $2E_A/k_B T_{MI}$ decreases and its limiting value at $E_A=0$ is approximately 1.3. Even if we take the limits of uncertainty of both T_{MI} and E_A into consideration, it cannot be expected that $2E_A/k_B T_{MI}$ approaches zero. Though the definition of T_{MI} used in this paper is rather arbitrary, the above conclusion does not change if T_{MI} is defined in a different way. For example, The temperature difference between the peak in $|d(\ln \sigma_o)/d(T)|$ and that in $|d(\ln \sigma_o)/d(1/T)|$ does not exceed 0.2 K. We have not extended measurements on $(TMTSF)_2PF_6$ to higher pressure but it is expected that the ratio remains finite at high pressure as in $(TMTSF)_2AsF_6$.

According to the mean-field theory, maxima of the density of states in the SDW

Fig.1 $|d(\ln \sigma_o)/d(1/T)|$ vs. temperature.
(σ_o : ohmic conductivity)

Fig.2 Metal-insulator transition temperature T_{MI} and activation energy E_A under pressure.

Fig.3. Ratio $2E_A/k_B T_{MI}$ vs. E_A .

state are located at $E=\pm(\Delta_0+\varepsilon_0)$. Their magnitudes decrease with increasing ε_0 . On the other hand, the density of states at $E=\pm(\Delta_0-\varepsilon_0)$ is finite irrespective of ε_0 . Thus almost all the carriers are excited between the top of occupied band and bottom of unoccupied band; the activation energy E_A obtained below 2 K is approximately equal to $\Delta_0-\varepsilon_0$.

If there are impurity levels between occupied and unoccupied bands, E_A cannot be determined from the Arrhenius plot, or it would be smaller than $\Delta_0-\varepsilon_0$ even if the Arrhenius plot is approximated by a linear curve. In fact, we observed non-linear curves in some $(\text{TMTSF})_2\text{PF}_6$ samples. In such cases, we obtained E_A from $\sigma_0-\sigma_i$ instead of σ_0 , where σ_i is a constant independent of temperature. It was assumed that the carriers provided by impurities contribute to σ_i . These E_A values are in agreement with those determined from other samples which show the regular linear Arrhenius curves.

We found that the limiting value of $2E_A/k_B T_{M1}$ is 1.3, which is close to 1.4 calculated by Yamaji [3]. Therefore, T_{M1} determined experimentally is not equal to T_{SDW} but lower than T_{SDW} .

In several samples of both $(\text{TMTSF})_2\text{AsF}_6$ and $(\text{TMTSF})_2\text{PF}_6$, non-linear conduction was observed above T_{M1} . In some of them a finite threshold field was found and it decreases with increasing temperature and vanishes at a temperature slightly higher than T_{M1} . We expect that T_{SDW} can be determined by extrapolation of the threshold field to zero.

References

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